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The crystal structure of 2-bromoisophthalic acid, $C_8H_5BrO_4$

Table 1: Data collection and handling.

Crystal:	Colorless block
Size:	$0.3 \times 0.25 \times 0.1$ mm
Wavelength:	Mo $K\alpha$ radiation (0.71073 Å)
μ :	5.10 mm^{-1}
Diffractometer, scan mode:	Bruker APEX-II, φ and ω -scans
θ_{max} , completeness:	26.5° , >99%
$N(hkl)_{\text{measured}}$, $N(hkl)_{\text{unique}}$, R_{int} :	8569, 1646, 0.034
Criterion for I_{obs} , $N(hkl)_{\text{gt}}$:	$I_{\text{obs}} > 2 \sigma(I_{\text{obs}})$, 1490
$N(\text{param})_{\text{refined}}$:	120
Programs:	Bruker programs [1], SHELX [2], OLEX2 [3, 4]

<https://doi.org/10.1515/ncrs-2019-0457>

Received June 30, 2019; accepted July 25, 2019; available online September 11, 2019

Abstract

$C_8H_5BrO_4$, triclinic, $P\bar{1}$ (no. 2), $a = 4.8161(3)$ Å, $b = 7.3727(5)$ Å, $c = 12.1230(7)$ Å, $\alpha = 81.004(3)^\circ$, $\beta = 78.897(3)^\circ$, $\gamma = 72.829(3)^\circ$, $V = 401.30(4)$ Å³, $Z = 2$, $R_{\text{gt}}(F) = 0.0201$, $wR_{\text{ref}}(F^2) = 0.0479$, $T = 150(2)$ K.

CCDC no.: 1941305

The crystal structure is shown in the figure. Table 1 contains crystallographic data and Table 2 contains the list of the atoms including atomic coordinates and displacement parameters.

Source of materials

All of reagents are commercial resource and used as received. The title organic molecule was recrystallized as follows: under stirring, to a THF solution (10 mL), 1 mmol 2-bromoisophthalic acid (0.245 g) was added and heated at 50°C for 1 h. The filtrate let evaporate in air at room temperature. A large number of colorless crystals were obtained after several days, washed with a small amount of water and air-dried.

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Table 2: Fractional atomic coordinates and isotropic or equivalent isotropic displacement parameters (Å²).

Atom	<i>x</i>	<i>y</i>	<i>z</i>	$U_{\text{iso}}^*/U_{\text{eq}}$
Br1	0.76797(5)	0.08612(3)	0.823044(18)	0.02095(8)
C1	0.5975(4)	0.4959(3)	0.79963(16)	0.0114(4)
C2	0.5992(4)	0.3320(3)	0.75373(16)	0.0117(4)
C3	0.4436(4)	0.3504(3)	0.66412(17)	0.0125(4)
C4	0.2717(4)	0.5296(3)	0.62740(17)	0.0145(4)
H4	0.1610(4)	0.5414(3)	0.56848(17)	0.0174(5)*
C5	0.2597(5)	0.6911(3)	0.67535(18)	0.0162(4)
H5	0.1381(5)	0.8121(3)	0.65085(18)	0.0194(5)*
C6	0.4265(5)	0.6740(3)	0.75926(17)	0.0148(4)
H6	0.4250(5)	0.7852(3)	0.79004(17)	0.0178(5)*
C7	0.7764(4)	0.4919(3)	0.88843(17)	0.0128(4)
C8	0.4642(5)	0.1883(3)	0.59985(17)	0.0133(4)
O1	0.6806(3)	0.6476(2)	0.94095(13)	0.0187(3)
H1	0.792(3)	0.6424(18)	0.9876(17)	0.0280(5)*
O2	0.9923(3)	0.3629(2)	0.90761(13)	0.0185(3)
O3	0.6813(3)	0.0537(2)	0.58514(13)	0.0187(3)
O4	0.2260(3)	0.2132(2)	0.55388(13)	0.0197(3)
H4a	0.251(2)	0.123(2)	0.5151(19)	0.0295(5)*

Experimental details

All H-atoms from C atoms and O_{hydroxyl} atoms were positioned with idealized geometry and refined isotropically ($U_{\text{iso}}(\text{H}) = 1.2U_{\text{eq}}(\text{C})$ or $1.5U_{\text{eq}}(\text{O})$ for all H atoms) using a riding model with $\text{C}—\text{H} = 0.95$ Å and $\text{O}—\text{H} = 0.84$ Å.

Comment

Several crystal structures of bromine-substituted isophthalic acids or their derivatives have been reported,

such as 5-bromoisophthalic acid [5, 6], 5-amino-2,4,6-tribromoisophthalic acid [7], 4,6-dibromoisophthalic acid monohydrate [8], 4,4'-dibromo-1,1'-biphenyl-2,2',6,6'-tetracarboxylic acid [9], 2-bromobenzene-1,3,5-tricarboxylic acid monohydrate [10], 2,5-dibromoisophthalic acid monohydrate and 5-bromo-2-((2-methoxyphenyl)(phenyl)amino)isophthalic acid [11]. However, the crystal structure of 2-bromoisophthalic acid has not been reported anywhere. Thus, we herein report the crystal structure of the title compound.

As shown in the figure, the title compound, named 2-bromoisophthalic acid, with the molecule formula C₈H₅BrO₄, crystallizes in the triclinic space group *P* $\bar{1}$. All bond lengths and angles of the title compound are normal, compared with its analogues [5–11]. The benzene ring is nearly planar. The two carboxyl groups are not coplanar with the aforementioned ring. There are two kinds of O–H···O hydrogen bonds: one is O1–H1···O2, the other is O4–H4a···O3, with their D···A distances 2.6183(24) and 2.6722(23) Å, respectively. These hydrogen bonds link molecules to generate a one-dimensional chain.

Acknowledgements: This study was supported by Pei Ying Plan of SIVA (Z.30001.16.05.16.14) and Education Department of Highland Construction Action Plan of SIVA (Z.31008.17.06). Dr. G. Huang also thanks Chinese Academy of Cultural Heritage for his postdoctoral position.

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